IUCrData

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2-({6-[5-Methyl-1-(4-methylphenyl)-1*H*-1,2,3-triazol-4-yl]imidazo[2,1-*b*]thiazol-5-yl}methylidene)hydrazinecarbothioamide dimethylformamide 0.25-solvate

Gamal A. El-Hiti,[a]* Bakr F. Abdel-Wahab,[b,c] Mohammad Hayal Alotaibi,[d] Amany S. Hegazy[e] and Benson M. Kariuki[e]‡

[a]Cornea Research Chair, Department of Optometry, College of Applied Medical Sciences, King Saud University, PO Box 10219, Riyadh 11433, Saudi Arabia, [b]Department of Chemistry, College of Science and Humanities, Shaqra University, Duwadimi, Saudi Arabia, [c]Applied Organic Chemistry Department, National Research Centre, Dokki, Giza, Egypt, [d]National Center for Petrochemicals Technology, King Abdulaziz City for Science and Technology, PO Box 6086, Riyadh 11442, Saudi Arabia, and [e]School of Chemistry, Cardiff University, Main Building, Park Place, Cardiff CF10 3AT, UK. *Correspondence e-mail: gelhiti@ksu.edu.sa

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‡ Additional corresponding author, e-mail: kariukib@cardiff.ac.uk.

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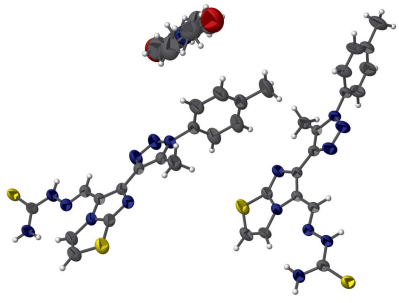
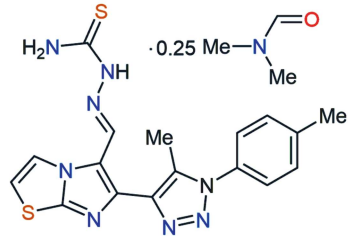
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title solvate, $C_{17}H_{16}N_8S_2\cdot0.25C_3H_7NO$, consists of two $C_{17}H_{16}N_8S_2$ molecules and a dimethylformamide molecule disordered about a crystallographic inversion centre. Both triazole molecules feature an intramolecular C—H···N interaction, which generates an *S*(6) ring in each case. In the crystal, the components are linked by N—H···N and N—H···S hydrogen bonds to form [001] chains, which are cross-linked by weak C—H···O, C—H···N and C—H···S interactions.

3D view



Chemical scheme



Structure description

Heterocyclic compounds that contain the thiosemicarbazone residue show a number of biological applications (see, for example, Salman *et al.*, 2016; Yusuf & Jain, 2014; Abdel-Wahab *et al.*, 2017). As part of our studies in this area, we now describe the synthesis and structure of the title solvate.

The asymmetric unit consists of two independent $C_{17}H_{16}N_8S_2$ molecules (*A* and *B*) and half a molecule of dimethyl formamide solvent disordered about an inversion centre (Fig. 1). In molecule *A*, the dihedral angles between the triazole ring and the toluyl and imidazole rings are 81.1 (2) and 8.5 (2)°, respectively. Equivalent values for molecule *B*

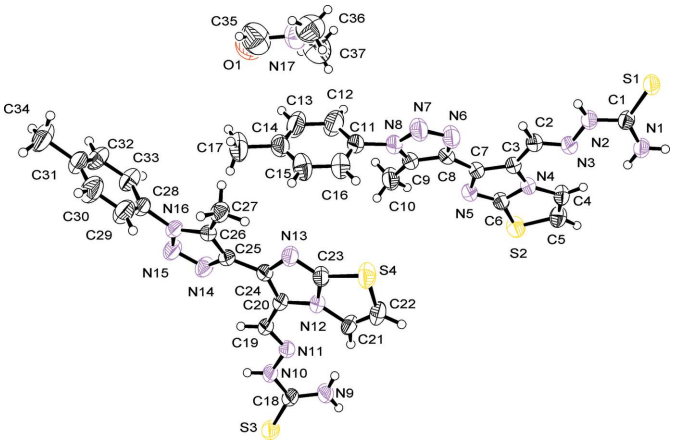


Figure 1
The molecular structure of the title solvate showing 50% displacement ellipsoids.

are 58.8 (2) and 13.83 (19)°, respectively. Both molecules feature an intramolecular C—H···N interaction, which generates an *S*(6) ring in each case.

In the crystal, N—H···S and N—H···N hydrogen bonds (Table 1) with N···*X* distances in the range 3.024 (4)–3.502 (3) Å lead to the formation of [001] chains (Fig. 2), which are cross-linked by weak C—H···N, C—H···O and C—H···S interactions.

Synthesis and crystallization

The title compound, which crystallized as a 0.25 dimethylformamide solvate, was synthesized from a mixture of 6-[5-methyl-1-(4-tolyl)-1*H*-1,2,3-triazol-4-yl]imidazo[2,1-*b*]thia-]thiazole-5-carbaldehyde and thiosemicarbazide in boiling dry ethanol for 4 h under catalytic acidic conditions (glacial acetic acid). The reaction mixture was left to cool to room temperature and the solid produced was collected, washed with ethanol and recrystallized as yellow plates from dimethylformamide solution, m.p. 229–230°C (Abdel-Wahab *et al.*, 2017).

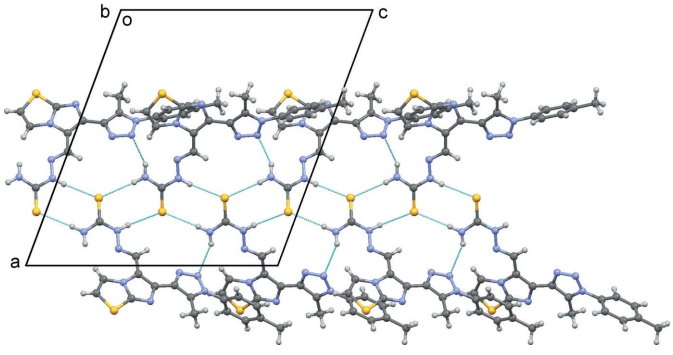


Figure 2
A view of a segment of the crystal structure viewed down the *b* axis. Intermolecular contacts are shown as blue dotted lines.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10*A*···N5	0.96	2.39	3.074 (4)	128
C27—H27*A*···N13	0.96	2.41	3.082 (4)	127
N1—H1*A*···N7^{i}	0.86	2.62	3.200 (4)	126
N1—H1*B*···S3^{ii}	0.86	2.62	3.470 (3)	172
N2—H2*A*···S3^{iii}	0.86	2.65	3.502 (3)	174
N9—H9*A*···N15^{i}	0.86	2.34	3.024 (4)	136
N9—H9*B*···S1^{iv}	0.86	2.64	3.433 (3)	154
N10—H10···S1^{v}	0.86	2.55	3.388 (3)	166
C5—H5···O1^{vi}	0.93	2.59	3.472 (10)	158
C36—H36*C*···S3^{vii}	0.96	2.72	3.536 (14)	143
C37—H37*B*···N6^{viii}	0.96	2.45	3.111 (11)	126
C37—H37*C*···S3^{ix}	0.96	2.75	3.706 (13)	175

Symmetry codes: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $x-1, y, z-1$; (iii) $x-1, -y+\frac{1}{2}, z-\frac{1}{2}$; (iv) $x+1, -y+\frac{1}{2}, z+\frac{1}{2}$; (v) $x+1, y, z+1$; (vi) $x, y, z-1$; (vii) $x-1, y, z$; (viii) $-x, y-\frac{1}{2}, -z+\frac{3}{2}$; (ix) $-x+1, -y, -z+2$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$4C_{17}H_{16}N_8S_2·C_3H_7NO$
M_r	1659.08
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, *b*, *c* (Å)	18.3427 (14), 13.5855 (10), 16.9385 (12)
β (°)	110.393 (9)
V (Å^3)	3956.4 (5)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.29
Crystal size (mm)	0.38 × 0.21 × 0.19
Data collection	
Diffractometer	Agilent SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.996, 0.998
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22546, 9646, 5318
R_{int}	0.049
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.702
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.064, 0.181, 1.04
No. of reflections	9646
No. of parameters	533
No. of restraints	61
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.29

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXS2013* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *CHEMDRAW Ultra* (Cambridge Soft, 2001).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

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full crystallographic data

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Crystal data

$4C_{17}H_{16}N_8S_2{\cdot}C_3H_7NO$
M_r = 1659.08
Monoclinic, $P2_1/c$
a = 18.3427 (14) Å
b = 13.5855 (10) Å
c = 16.9385 (12) Å
β = 110.393 (9)°
V = 3956.4 (5) Å^3
Z = 2
$F(000)$ = 1728
D_x = 1.393 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4302 reflections
θ = 3.8–25.9°
μ = 0.29 mm^{-1}
T = 296 K
Plate, yellow
0.38 × 0.21 × 0.19 mm

Data collection

Agilent SuperNova, Dual, Cu at zero, Atlas diffractometer
ω scans
Absorption correction: gaussian (CrysAlisPro; Agilent, 2014)
T_{min} = 0.996, T_{max} = 0.998
22546 measured reflections
9646 independent reflections
5318 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 30.0°, θ_{min} = 2.4°
h = −24→23
k = −18→14
l = −23→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.181
S = 1.04
9646 reflections
533 parameters
61 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.060P)^2 + 2.4742P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Special details

Experimental. Numerical absorption correction based on gaussian integration over a multifaceted crystal model Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. All hydrogen atoms were placed in calculated positions and refined using a riding model. Methyl C—H bonds were fixed at 0.96 Å, with displacement parameters 1.5 times U_{eq}(C), and were allowed to spin about the C—C/C—N bonds. N—H bonds were fixed at 0.86 Å and sp^2 C—H distances were set to 0.93 Å and their U(iso) set to 1.2 times the U_{eq} for the atoms to which they are bonded. The DMF solvent molecule is diordered about a crystallographic inversion centre.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	−0.17220 (19)	0.2265 (2)	0.22798 (18)	0.0442 (7)	
C2	−0.03664 (18)	0.1621 (2)	0.42338 (19)	0.0448 (7)	
H2	−0.0605	0.1912	0.4578	0.054*	
C3	0.03317 (17)	0.1064 (2)	0.45952 (18)	0.0416 (7)	
C4	0.0536 (2)	0.0284 (3)	0.3275 (2)	0.0526 (9)	
H4	0.0134	0.0543	0.2821	0.063*	
C5	0.1076 (2)	−0.0338 (3)	0.3208 (2)	0.0578 (9)	
H5	0.1087	−0.0562	0.2693	0.069*	
C6	0.12846 (19)	0.0026 (2)	0.46744 (19)	0.0452 (7)	
C7	0.08037 (17)	0.0885 (2)	0.54231 (18)	0.0425 (7)	
C8	0.07685 (17)	0.1309 (3)	0.61939 (19)	0.0465 (8)	
C9	0.12373 (18)	0.1110 (3)	0.70155 (19)	0.0481 (8)	
C10	0.1875 (2)	0.0397 (3)	0.7394 (2)	0.0657 (10)	
H10A	0.1948	0.0001	0.6958	0.099*	
H10B	0.1744	−0.0020	0.7783	0.099*	
H10C	0.2347	0.0747	0.7687	0.099*	
C11	0.1323 (2)	0.1929 (3)	0.8362 (2)	0.0583 (10)	
C12	0.1221 (3)	0.1250 (5)	0.8906 (3)	0.118 (2)	
H12	0.0917	0.0695	0.8706	0.142*	
C13	0.1585 (3)	0.1405 (5)	0.9772 (3)	0.113 (2)	
H13	0.1510	0.0947	1.0144	0.136*	
C14	0.2041 (2)	0.2197 (3)	1.0089 (2)	0.0658 (11)	
C15	0.2145 (3)	0.2844 (3)	0.9527 (2)	0.0710 (11)	
H15	0.2467	0.3385	0.9727	0.085*	
C16	0.1788 (2)	0.2725 (3)	0.8668 (2)	0.0651 (10)	
H16	0.1864	0.3187	0.8299	0.078*	
C17	0.2440 (3)	0.2316 (4)	1.1029 (2)	0.0878 (15)	
H17A	0.2992	0.2261	1.1168	0.132*	
H17B	0.2263	0.1812	1.1316	0.132*	
H17C	0.2317	0.2951	1.1198	0.132*	
C18	0.69548 (19)	0.2204 (3)	0.92434 (19)	0.0472 (8)	
C19	0.55451 (17)	0.3166 (2)	0.99815 (18)	0.0427 (7)	
H19	0.5798	0.3042	1.0552	0.051*	

C20	0.48128 (17)	0.3667 (2)	0.97028 (17)	0.0403 (7)
C21	0.4551 (2)	0.3982 (3)	0.81034 (18)	0.0494 (8)
H21	0.4974	0.3692	0.8012	0.059*
C22	0.3979 (2)	0.4438 (3)	0.7517 (2)	0.0603 (10)
H22	0.3956	0.4497	0.6962	0.072*
C23	0.37887 (19)	0.4471 (3)	0.88651 (18)	0.0457 (8)
C24	0.43284 (17)	0.3984 (2)	1.01217 (17)	0.0406 (7)
C25	0.44181 (17)	0.3852 (3)	1.10053 (18)	0.0430 (7)
C26	0.40246 (17)	0.4329 (2)	1.14538 (17)	0.0409 (7)
C27	0.3392 (2)	0.5065 (3)	1.1218 (2)	0.0523 (9)
H27A	0.3301	0.5290	1.0655	0.078*
H27B	0.3538	0.5612	1.1600	0.078*
H27C	0.2926	0.4770	1.1247	0.078*
C28	0.41642 (19)	0.4155 (3)	1.29788 (18)	0.0481 (8)
C29	0.4243 (3)	0.5090 (3)	1.3295 (2)	0.0717 (12)
H29	0.4406	0.5597	1.3026	0.086*
C30	0.4079 (3)	0.5276 (4)	1.4015 (3)	0.0833 (14)
H30	0.4132	0.5914	1.4227	0.100*
C31	0.3838 (2)	0.4544 (3)	1.4426 (2)	0.0651 (11)
C32	0.3755 (2)	0.3616 (3)	1.4096 (2)	0.0644 (11)
H32	0.3596	0.3110	1.4368	0.077*
C33	0.3905 (2)	0.3413 (3)	1.3360 (2)	0.0592 (10)
H33	0.3830	0.2783	1.3131	0.071*
C34	0.3650 (3)	0.4757 (4)	1.5213 (3)	0.1001 (17)
H34A	0.3132	0.5016	1.5056	0.150*
H34B	0.4013	0.5230	1.5553	0.150*
H34C	0.3687	0.4160	1.5527	0.150*
N1	−0.13188 (16)	0.2004 (2)	0.18044 (16)	0.0546 (8)
H1A	−0.0849	0.1796	0.2033	0.066*
H1B	−0.1525	0.2043	0.1265	0.066*
N2	−0.13701 (15)	0.2189 (2)	0.31172 (15)	0.0484 (7)
H2A	−0.1583	0.2432	0.3453	0.058*
N3	−0.06606 (15)	0.1716 (2)	0.34324 (16)	0.0466 (6)
N4	0.06536 (14)	0.0494 (2)	0.41195 (15)	0.0426 (6)
N5	0.13947 (15)	0.0238 (2)	0.54691 (15)	0.0478 (7)
N6	0.02709 (18)	0.2052 (3)	0.61998 (18)	0.0678 (9)
N7	0.04052 (19)	0.2341 (3)	0.69742 (19)	0.0737 (10)
N8	0.09920 (16)	0.1767 (3)	0.74714 (16)	0.0575 (8)
N9	0.65336 (16)	0.2177 (2)	0.84265 (16)	0.0593 (8)
H9A	0.6050	0.2340	0.8256	0.071*
H9B	0.6744	0.1998	0.8069	0.071*
N10	0.65883 (14)	0.2492 (2)	0.97685 (15)	0.0485 (7)
H10	0.6813	0.2429	1.0304	0.058*
N11	0.58528 (14)	0.2886 (2)	0.94434 (15)	0.0439 (6)
N12	0.44408 (14)	0.39909 (19)	0.88760 (14)	0.0413 (6)
N13	0.36887 (15)	0.4480 (2)	0.95978 (15)	0.0501 (7)
N14	0.49389 (16)	0.3208 (2)	1.15125 (17)	0.0565 (8)
N15	0.48920 (16)	0.3257 (2)	1.22687 (16)	0.0579 (8)

N16	0.43392 (14)	0.3939 (2)	1.22340 (15)	0.0466 (7)	
S1	−0.26434 (5)	0.26826 (9)	0.18941 (5)	0.0621 (3)	
S2	0.17525 (6)	−0.06895 (8)	0.41659 (6)	0.0609 (3)	
S3	0.78985 (5)	0.18878 (9)	0.96231 (5)	0.0624 (3)	
S4	0.32750 (6)	0.49162 (9)	0.78729 (6)	0.0676 (3)	
C35	0.0467 (9)	−0.0002 (12)	1.0935 (5)	0.134 (4)	0.5
H35	0.0527	0.0519	1.1309	0.161*	0.5
C36	−0.0348 (7)	0.0759 (10)	0.9677 (9)	0.108 (3)	0.5
H36A	−0.0369	0.0804	0.9104	0.163*	0.5
H36B	−0.0078	0.1321	0.9987	0.163*	0.5
H36C	−0.0867	0.0741	0.9690	0.163*	0.5
C37	0.0126 (7)	−0.0813 (7)	0.9478 (8)	0.115 (4)	0.5
H37A	0.0088	−0.0562	0.8935	0.173*	0.5
H37B	−0.0262	−0.1311	0.9410	0.173*	0.5
H37C	0.0633	−0.1091	0.9749	0.173*	0.5
N17	0.0000	0.0000	1.0000	0.0897 (16)	
O1	0.0702 (6)	−0.0692 (9)	1.1073 (6)	0.149 (3)	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0496 (18)	0.0463 (19)	0.0370 (16)	0.0037 (15)	0.0155 (14)	0.0063 (14)
C2	0.0438 (17)	0.050 (2)	0.0386 (16)	−0.0014 (15)	0.0118 (14)	−0.0023 (15)
C3	0.0374 (16)	0.050 (2)	0.0360 (15)	−0.0007 (14)	0.0108 (13)	0.0000 (14)
C4	0.058 (2)	0.060 (2)	0.0361 (16)	0.0022 (18)	0.0110 (15)	−0.0010 (16)
C5	0.070 (2)	0.061 (2)	0.0421 (18)	0.003 (2)	0.0189 (17)	−0.0055 (17)
C6	0.0429 (17)	0.048 (2)	0.0413 (16)	−0.0011 (15)	0.0107 (14)	−0.0002 (15)
C7	0.0359 (15)	0.052 (2)	0.0364 (15)	−0.0026 (15)	0.0091 (13)	0.0015 (14)
C8	0.0337 (15)	0.063 (2)	0.0392 (16)	−0.0046 (16)	0.0086 (13)	−0.0023 (15)
C9	0.0401 (17)	0.064 (2)	0.0379 (16)	−0.0072 (16)	0.0106 (14)	−0.0042 (16)
C10	0.067 (2)	0.077 (3)	0.0452 (19)	0.005 (2)	0.0089 (18)	0.0041 (19)
C11	0.0456 (19)	0.090 (3)	0.0392 (17)	0.000 (2)	0.0142 (15)	−0.0086 (19)
C12	0.130 (4)	0.172 (6)	0.054 (3)	−0.093 (4)	0.033 (3)	−0.017 (3)
C13	0.124 (4)	0.168 (6)	0.047 (2)	−0.064 (4)	0.031 (3)	−0.003 (3)
C14	0.058 (2)	0.087 (3)	0.048 (2)	0.010 (2)	0.0137 (18)	−0.013 (2)
C15	0.081 (3)	0.065 (3)	0.053 (2)	0.010 (2)	0.005 (2)	−0.012 (2)
C16	0.079 (3)	0.059 (2)	0.049 (2)	0.010 (2)	0.0119 (19)	−0.0013 (18)
C17	0.095 (3)	0.106 (4)	0.048 (2)	0.023 (3)	0.007 (2)	−0.012 (2)
C18	0.0462 (18)	0.061 (2)	0.0389 (16)	0.0017 (16)	0.0200 (14)	−0.0028 (15)
C19	0.0394 (16)	0.058 (2)	0.0328 (15)	−0.0001 (15)	0.0151 (13)	−0.0003 (14)
C20	0.0417 (16)	0.0494 (19)	0.0318 (14)	−0.0009 (15)	0.0152 (13)	−0.0012 (13)
C21	0.059 (2)	0.059 (2)	0.0335 (16)	−0.0019 (18)	0.0212 (15)	0.0017 (15)
C22	0.077 (2)	0.070 (3)	0.0333 (16)	0.000 (2)	0.0186 (17)	0.0023 (17)
C23	0.0462 (18)	0.053 (2)	0.0349 (15)	0.0062 (16)	0.0104 (13)	−0.0017 (15)
C24	0.0353 (15)	0.051 (2)	0.0349 (15)	0.0010 (14)	0.0121 (13)	−0.0024 (14)
C25	0.0352 (15)	0.060 (2)	0.0361 (15)	0.0015 (15)	0.0147 (13)	0.0005 (15)
C26	0.0331 (15)	0.056 (2)	0.0342 (15)	−0.0019 (14)	0.0121 (12)	−0.0017 (14)
C27	0.0515 (19)	0.064 (2)	0.0439 (17)	0.0124 (18)	0.0201 (16)	0.0016 (16)

C28	0.0457 (18)	0.067 (2)	0.0345 (15)	0.0041 (17)	0.0182 (14)	0.0021 (16)
C29	0.099 (3)	0.072 (3)	0.057 (2)	−0.026 (2)	0.043 (2)	−0.010 (2)
C30	0.117 (4)	0.080 (3)	0.068 (3)	−0.026 (3)	0.051 (3)	−0.025 (2)
C31	0.072 (3)	0.088 (3)	0.0421 (19)	0.003 (2)	0.0283 (18)	0.002 (2)
C32	0.083 (3)	0.069 (3)	0.055 (2)	0.016 (2)	0.041 (2)	0.020 (2)
C33	0.078 (3)	0.057 (2)	0.052 (2)	0.013 (2)	0.0341 (19)	0.0091 (18)
C34	0.128 (4)	0.131 (4)	0.059 (3)	−0.007 (4)	0.055 (3)	−0.015 (3)
N1	0.0481 (16)	0.079 (2)	0.0369 (14)	0.0186 (15)	0.0151 (12)	0.0111 (14)
N2	0.0440 (15)	0.0634 (19)	0.0361 (13)	0.0115 (14)	0.0118 (12)	0.0010 (13)
N3	0.0405 (14)	0.0556 (18)	0.0411 (14)	0.0055 (13)	0.0110 (12)	0.0055 (13)
N4	0.0382 (13)	0.0489 (16)	0.0365 (13)	−0.0018 (12)	0.0077 (11)	−0.0007 (12)
N5	0.0401 (14)	0.0602 (18)	0.0395 (14)	0.0012 (13)	0.0093 (12)	−0.0003 (13)
N6	0.0574 (18)	0.097 (3)	0.0430 (16)	0.0199 (18)	0.0102 (14)	−0.0072 (17)
N7	0.0565 (19)	0.112 (3)	0.0465 (17)	0.020 (2)	0.0109 (15)	−0.0134 (18)
N8	0.0457 (16)	0.087 (2)	0.0377 (14)	0.0020 (16)	0.0122 (13)	−0.0061 (15)
N9	0.0418 (15)	0.098 (2)	0.0383 (14)	0.0054 (16)	0.0139 (12)	−0.0152 (15)
N10	0.0391 (14)	0.075 (2)	0.0326 (12)	0.0078 (14)	0.0134 (11)	−0.0015 (13)
N11	0.0361 (13)	0.0590 (18)	0.0361 (13)	0.0038 (13)	0.0121 (11)	−0.0021 (12)
N12	0.0450 (14)	0.0473 (16)	0.0315 (12)	−0.0004 (12)	0.0132 (11)	−0.0010 (11)
N13	0.0471 (15)	0.0671 (19)	0.0358 (13)	0.0093 (14)	0.0139 (12)	0.0004 (13)
N14	0.0513 (16)	0.079 (2)	0.0435 (15)	0.0221 (16)	0.0219 (13)	0.0120 (15)
N15	0.0524 (17)	0.084 (2)	0.0414 (15)	0.0236 (16)	0.0219 (13)	0.0123 (15)
N16	0.0397 (14)	0.0672 (19)	0.0360 (13)	0.0065 (14)	0.0172 (11)	0.0045 (13)
S1	0.0485 (5)	0.0994 (8)	0.0374 (4)	0.0228 (5)	0.0138 (4)	0.0097 (5)
S2	0.0590 (6)	0.0653 (6)	0.0541 (5)	0.0121 (5)	0.0144 (4)	−0.0079 (5)
S3	0.0440 (5)	0.0991 (8)	0.0470 (5)	0.0136 (5)	0.0195 (4)	−0.0007 (5)
S4	0.0719 (6)	0.0821 (8)	0.0406 (5)	0.0197 (6)	0.0090 (4)	0.0082 (5)
C35	0.129 (6)	0.120 (6)	0.132 (6)	−0.007 (6)	0.020 (5)	0.024 (6)
C36	0.103 (8)	0.104 (8)	0.122 (8)	0.017 (7)	0.044 (7)	0.012 (7)
C37	0.120 (8)	0.086 (7)	0.127 (8)	0.009 (6)	0.026 (7)	−0.029 (7)
N17	0.102 (4)	0.081 (4)	0.081 (3)	−0.007 (3)	0.025 (3)	−0.001 (3)
O1	0.139 (7)	0.164 (8)	0.136 (7)	0.033 (7)	0.037 (6)	−0.004 (7)

Geometric parameters (Å, º)

C1—N1	1.317 (4)	C20—C24	1.385 (4)
C1—N2	1.342 (4)	C20—N12	1.398 (4)
C1—S1	1.684 (3)	C21—C22	1.321 (5)
C2—N3	1.281 (4)	C21—N12	1.392 (4)
C2—C3	1.429 (4)	C22—S4	1.730 (4)
C3—C7	1.389 (4)	C23—N13	1.316 (4)
C3—N4	1.389 (4)	C23—N12	1.357 (4)
C4—C5	1.338 (5)	C23—S4	1.724 (3)
C4—N4	1.399 (4)	C24—N13	1.375 (4)
C5—S2	1.731 (4)	C24—C25	1.459 (4)
C6—N5	1.321 (4)	C25—N14	1.358 (4)
C6—N4	1.367 (4)	C25—C26	1.379 (4)
C6—S2	1.715 (3)	C26—N16	1.352 (4)

C7—N5	1.376 (4)	C26—C27	1.477 (4)
C7—C8	1.449 (4)	C28—C29	1.366 (5)
C8—N6	1.363 (4)	C28—C33	1.368 (5)
C8—C9	1.384 (4)	C28—N16	1.436 (4)
C9—N8	1.355 (4)	C29—C30	1.377 (5)
C9—C10	1.483 (5)	C30—C31	1.373 (6)
C11—C12	1.361 (6)	C31—C32	1.365 (6)
C11—C16	1.363 (5)	C31—C34	1.516 (5)
C11—N8	1.434 (4)	C32—C33	1.395 (5)
C12—C13	1.400 (6)	N2—N3	1.381 (3)
C13—C14	1.353 (7)	N6—N7	1.308 (4)
C14—C15	1.356 (6)	N7—N8	1.358 (4)
C14—C17	1.512 (5)	N10—N11	1.376 (3)
C15—C16	1.382 (5)	N14—N15	1.315 (3)
C18—N9	1.330 (4)	N15—N16	1.360 (4)
C18—N10	1.346 (4)	C35—O1	1.025 (16)
C18—S3	1.679 (3)	C35—N17	1.516 (8)
C19—N11	1.285 (4)	C36—N17	1.235 (12)
C19—C20	1.431 (4)	C37—N17	1.482 (6)

N1—C1—N2	117.4 (3)	C20—C24—C25	128.6 (3)
N1—C1—S1	123.7 (2)	N14—C25—C26	110.0 (3)
N2—C1—S1	118.9 (2)	N14—C25—C24	122.1 (3)
N3—C2—C3	119.4 (3)	C26—C25—C24	127.9 (3)
C7—C3—N4	104.3 (3)	N16—C26—C25	103.1 (3)
C7—C3—C2	132.5 (3)	N16—C26—C27	123.8 (3)
N4—C3—C2	123.1 (3)	C25—C26—C27	133.0 (3)
C5—C4—N4	111.1 (3)	C29—C28—C33	120.5 (3)
C4—C5—S2	113.9 (3)	C29—C28—N16	120.6 (3)
N5—C6—N4	113.1 (3)	C33—C28—N16	118.9 (3)
N5—C6—S2	135.2 (3)	C28—C29—C30	119.5 (4)
N4—C6—S2	111.7 (2)	C31—C30—C29	121.6 (4)
N5—C7—C3	111.8 (3)	C32—C31—C30	118.1 (3)
N5—C7—C8	119.0 (3)	C32—C31—C34	120.6 (4)
C3—C7—C8	129.2 (3)	C30—C31—C34	121.3 (4)
N6—C8—C9	108.7 (3)	C31—C32—C33	121.3 (4)
N6—C8—C7	122.8 (3)	C28—C33—C32	119.0 (4)
C9—C8—C7	128.4 (3)	C1—N2—N3	119.0 (2)
N8—C9—C8	103.4 (3)	C2—N3—N2	116.7 (3)
N8—C9—C10	123.5 (3)	C6—N4—C3	106.8 (2)
C8—C9—C10	133.1 (3)	C6—N4—C4	113.6 (3)
C12—C11—C16	119.7 (3)	C3—N4—C4	139.5 (3)
C12—C11—N8	120.1 (4)	C6—N5—C7	104.1 (3)
C16—C11—N8	120.0 (3)	N7—N6—C8	109.7 (3)
C11—C12—C13	118.7 (5)	N6—N7—N8	106.3 (3)
C14—C13—C12	122.5 (5)	C9—N8—N7	111.9 (3)
C13—C14—C15	117.1 (4)	C9—N8—C11	126.7 (3)
C13—C14—C17	120.5 (4)	N7—N8—C11	121.2 (3)

C15—C14—C17	122.3 (4)	C18—N10—N11	119.6 (2)
C14—C15—C16	122.1 (4)	C19—N11—N10	116.3 (2)
C11—C16—C15	119.8 (4)	C23—N12—C21	114.0 (3)
N9—C18—N10	116.9 (3)	C23—N12—C20	106.6 (2)
N9—C18—S3	122.7 (2)	C21—N12—C20	139.4 (3)
N10—C18—S3	120.4 (2)	C23—N13—C24	103.7 (2)
N11—C19—C20	120.0 (3)	N15—N14—C25	108.3 (3)
C24—C20—N12	103.8 (3)	N14—N15—N16	107.1 (2)
C24—C20—C19	132.5 (3)	C26—N16—N15	111.5 (2)
N12—C20—C19	123.7 (2)	C26—N16—C28	129.0 (3)
C22—C21—N12	111.4 (3)	N15—N16—C28	119.5 (2)
C21—C22—S4	114.0 (2)	C6—S2—C5	89.64 (17)
N13—C23—N12	113.8 (3)	C23—S4—C22	89.28 (16)
N13—C23—S4	135.0 (3)	O1—C35—N17	106.2 (12)
N12—C23—S4	111.2 (2)	C36—N17—C37	121.4 (7)
N13—C24—C20	112.2 (2)	C36—N17—C35	118.7 (8)
N13—C24—C25	119.2 (2)	C37—N17—C35	118.3 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10*A*···N5	0.96	2.39	3.074 (4)	128
C27—H27*A*···N13	0.96	2.41	3.082 (4)	127
N1—H1*A*···N7^{i}	0.86	2.62	3.200 (4)	126
N1—H1*B*···S3^{ii}	0.86	2.62	3.470 (3)	172
N2—H2*A*···S3^{iii}	0.86	2.65	3.502 (3)	174
N9—H9*A*···N15^{i}	0.86	2.34	3.024 (4)	136
N9—H9*B*···S1^{iv}	0.86	2.64	3.433 (3)	154
N10—H10···S1^{v}	0.86	2.55	3.388 (3)	166
C5—H5···O1^{vi}	0.93	2.59	3.472 (10)	158
C36—H36*C*···S3^{vii}	0.96	2.72	3.536 (14)	143
C37—H37*B*···N6^{viii}	0.96	2.45	3.111 (11)	126
C37—H37*C*···S3^{ix}	0.96	2.75	3.706 (13)	175

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (ii) *x*−1, *y*, *z*−1; (iii) *x*−1, −*y*+1/2, *z*−1/2; (iv) *x*+1, −*y*+1/2, *z*+1/2; (v) *x*+1, *y*, *z*+1; (vi) *x*, *y*, *z*−1; (vii) *x*−1, *y*, *z*; (viii) −*x*, *y*−1/2, −*z*+3/2; (ix) −*x*+1, −*y*, −*z*+2.